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TECHNICAL MEMORANDUM 1474

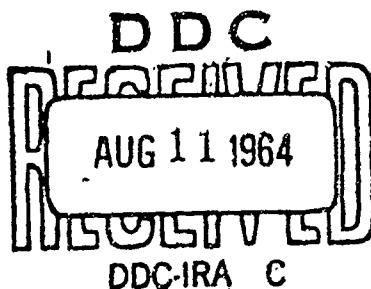
THE LOCATION
OF THE
CHAPMAN-JOUQUET PLANE
FOR A
GRANULAR EXPLOSIVE BY THE EFFECT OF
AREA INCREASE ON DETONATION VELOCITY

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AUGUST 1964

AMCMS NO. 5011.11.815001

COPY NO. 10



PICATINNY ARSENAL
DOVER, NEW JERSEY

Picatinny Arsenal Technical Memorandum 1474

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ABSTRACT

The detonation velocity for a granular mixture of potassium perchlorate and aluminum confined in a Lucite tube and an ideal detonation velocity calculated by the RUBY Computer Program have been used together with the observed reaction zone profile to estimate the position of the Chapman-Jouguet plane with respect to the plane at which reaction commences. This was done by extending Jones equation for effect of radial expansion on the detonation velocity to include the effect of covolume a function of volume. It was found that the CJ plane is about 0.9 cm. behind the plane at which reaction commences.

INTRODUCTION

A cylindrical charge of explosive detonates at a lower velocity than the ideal detonation velocity since the latter corresponds to a one dimensional process. The velocity decrease is governed by - the cross-sectional area increase at the Chapman-Jouguet (CJ) plane which depends on the confinement of the charge, the equation of state of the products, and the fluid dynamical equations. Jones (Ref. 1) has treated the case where a constant covolume equation of state may be assumed.

The granular explosive, considered in this report, has a long reaction zone, and doubles cross section in about a centimeter of length. Since a constant covolume can not be assumed for this case, the approach of Jones has been extended for covolume a function of volume. The equations developed permit determining area increase at the CJ plane as a function of the ratio of observed to ideal detonation velocity. This was done, using for the latter a theoretical value calculated with the RUBY Computer Program (Ref. 2). The area increase so derived was compared with the reaction zone profile to locate the CJ plane.

The granular explosive under study (Ref. 3-5) is a mixture of potassium perchlorate (22 micron) and atomized aluminum (15 micron) in the weight ratio 60/40. For convenience, this mixture is hereafter referred to as 60/40. The powder is loose-loaded (loading density 1.5 g/cm³) into a 3/8 inch-diameter axial hole in a 20 inch long, 3 inch diameter Lucite tube. Initiation is by a confined 0.36 gram tetryl pellet. A stable propagation profile at a constant velocity of about 900 m/sec is observed for the latter part of the tube. A typical stable profile is shown in Figure 1. Photographs showing the development and progression of the detonation are in References 3 and 5.

EQUATIONS

Jones (Ref. 1) derives the following system of equations in terms of the non-dimensional coordinates y , z , and other symbols defined below. Details are available in the cited reference. The introduction of the additional variable r means the system is short one equation for a unique solution. Jones formulation recasts the basic equations so that one variable \bar{y} can be considered a constant, thus permitting a particular solution.

Continuity

$$g U^{-1} = y r^{-2} \quad (1)$$

Momentum (from Bernoulli's equation)

$$z = 1 - y r^{-4} - 2 \int_{r_0}^r y r^{-5} dr \quad (2)$$

$$z_1 = 1 - y_1 r_1^{-4} - \frac{1}{2} \bar{y} (1 - r_1^{-4}) \quad (2a)$$

Energy

$$f(\epsilon, y, z) = U^{-2} (E - Q) = \frac{1}{2} z_0 (1 - \frac{y_0}{y}) - \int_{y_0}^y z dy \quad (3)$$

$$f(1, y_1, z_1) = \frac{1}{2} - \frac{y_1 z_1}{2} - \frac{1}{2} y_1^2 r_1^{-4} \quad (3a)$$

Chapman-Jouguet Condition

$$\left(\frac{\partial f}{\partial z} \right)_1 = r_1^{-4} \left\{ z_1 + \left(\frac{\partial f}{\partial y} \right)_1 \right\} \quad (4)$$

Equation of State

$$f(1, y, z) = \beta z, (y - b) - Q, U^{-2} \quad (5)$$

where

- r denotes the ratio of the radius of a stream tube at any point to that at the front. r^2 is a measure of radial area expansion.
- p denotes the pressure in excess of one atmosphere.
- U is the velocity of the detonation wave.
- Δ is the loading density of the explosive.
- ρ is the density of the fluid at any point beyond the shock wave front.
- q is the particle (fluid) velocity behind the front, relative to the detonation wave at rest.
- f is a dimensionless function of the non-dimensional coordinates y, z and the degree of reaction ϵ .
- E is the internal energy per unit mass relative to the initial site.
- Q is the chemical energy liberated per unit mass by the reaction.
- k is a parameter in the equation of state related to specific heat.
- b is a parameter in the equation of state related to covolume.

The subscript zero refers to conditions at the beginning of the reaction zone, that is behind the shock. The subscript one refers to conditions at the Chapman-Jouguet plane. No subscript indicates any point between these.

$$y = \Delta/\rho \quad z = p/U^2 \Delta$$

- \bar{y} is a mean value of y through the reaction zone defined in Eq. 11 which follows later. It is a new variable which must be approximated to obtain a solution.
- U_0 is the detonation velocity when there is no expansion of the reaction zone.

Jones treats k and b as constants and shows that the changes in detonation velocity in terms of radial expansion at the CJ plane are given by

$$\left(\frac{U_0}{U}\right)^2 = 1 + (\gamma_i^4 - 1) \left[\left(\frac{1 + \beta}{\beta(1 - \beta)} \right)^2 \left\{ 1 - \frac{1}{2} \bar{\gamma} (1 - \gamma_i^{-2}) \right\} \left\{ 1 - \frac{1}{2} \bar{\gamma} (1 + \gamma_i^{-2}) \right\} + \frac{b}{(1 - \beta)^2} \left(\frac{\bar{\gamma} - \beta}{\gamma_i^4} \right) \right] \quad (6)$$

This formula could not be used because the results calculated with it contradicted the assumption that the covolume was constant. The equation of state was then modified to treat b (related to covolume) as a linear function of y (the normalized density). This leads to a modification of Eq. 6 (to Eq. 9) as follows: Inserting Eq. 5 in 4 and then inserting Eq. 2a in the result leads to Eq. 7 below. Eq. 8 follows by using Eq. 7 in Eq. 2a. b' is the derivative of b with respect to y . Eqs. 7 and 8 are the analogues of Jones Eqs. 17 and 18.

$$(1 + 2\beta - b'\beta) \gamma_i = (1 + \beta(1 - b')) \left\{ \gamma_i^4 - \frac{1}{2} \bar{\gamma} (\gamma_i^4 - 1) \right\} + b\beta \quad (7)$$

$$(1 + 2\beta - b'\beta) \Xi_i = \beta \left(1 - \frac{1}{2} \bar{\gamma} (1 - \gamma_i^{-4}) \right) - b\beta \gamma_i^{-4} \quad (8)$$

If we substitute Eqs. 5, 7, and 8 into Eq. 3a we shall obtain a relation expressing U in terms of Q_1 , k , b , b' , r and $\bar{\gamma}$. By setting $U = U_0$ for $r = 1$ and eliminating Q_1 between the original and modified equation we arrive at the desired result for variable covolume, Eq. 9 below.

$$\left(\frac{U_0}{U}\right)^2 = \frac{\alpha \gamma_i^4 \beta^2 - 2b\beta\gamma_i + b^2\beta \gamma_i^{-4} - \delta}{\alpha - 2b\beta + b^2\beta - \delta} \quad (9)$$

where $\alpha = [1 + \beta(1 - b')] \left[1 + \frac{\beta(1 + 2\beta)}{(1 + 2\beta - b'\beta)} \right]$ $\beta = \beta^2 \frac{(1 + 2\beta - 2b'\beta)}{(1 + 2\beta - b'\beta)}$

$$\delta = (1 + 2\beta - b'\beta) \quad \gamma_i = 1 - \frac{1}{2} \bar{\gamma} (1 - \gamma_i^{-4})$$

Equation 9 reduces to Eq. 6 (Jones equation) for $b' = 0$ and $b = b_0$ (covolume for $r = 1$, considered constant). Note also that for $r_1 = 1$, $\gamma = 1$ that one obtains the expected $U = U_0$.

RESULTS

Equation 9 shows how the detonation velocity (U) depends on the radial expansion at the CJ plane (r_1). Conversely, using the observed U , and providing the other quantities in Eq. 9, one can find r_1 and locate the CJ plane from the observed reaction zone profile. The accuracy of the result of this calculation is limited by the variability in the experimental results and the assumptions necessary to specify the other quantities in the equation. In the paragraphs that follow, numerical values to be used in Eq. 9 are developed.

Since $b = a \Delta$, where a is the covolume per unit mass, and Δ is the loading density (1.5 g/cm^3), it follows that b is the covolume in units of $1/\Delta$. To calculate values of b , the RUBY Computer Program was used to calculate the CJ properties and those along an isentrope for the mixture under consideration. Since the program uses a Kistiakowsky-Wilson equation of state

$$\frac{PV}{nRT} = 1 + X e^{\beta X}$$

and the covolume form is $P(V - a) = nRT$,
the gaseous covolume is represented in RUBY notation by

$$\frac{nRT}{P} X e^{\beta X} = \frac{(\text{SUMN})(0.96494)/(T_{e.v})}{P_{\text{megabars}}} X e^{\beta X}$$

To this was added the volume per gram of explosive occupied by the two solid products, Al and Al_2O_3 . The covolumes obtained are tabulated below versus pressure and the RUBY density ratio RHOL0 which is the same as the y in Jones notation.

	RHOLO(y)	b
P_{CJ}	0.7080	0.6419
$P_{CJ}/\sqrt{10}$	1.1757	0.9933
$P_{CJ}/10$	2.0554	1.5433

These values were found to be fitted very well by the straight line equation

$$b = \frac{y}{1.5} + 0.175 \quad (10)$$

Thus, the value $(1.5)^{-1} = 0.6667$ is appropriate for the derivative b' .

The quantity, $k = \frac{C_V}{R}$, in the equation of state is the ratio of the specific heat from $E = C_V T$ to the gas constant from $p(V - a) = RT$. The value of k was calculated for those explosive products predicted by the RUBY program at the CJ point. Solid products were included in the weighted average for the specific heat calculation, but not in that for the gas constant. The value $k = 7.935$ resulted. No significant change from this value occurred for the products corresponding to a pressure drop along the isentrope to $1/10$ the CJ value. Thus, k was treated as a constant in the derivation of Eq. 9.

The quantity \bar{y} is defined in the Jones derivation as

$$\bar{y} = \frac{\int_{r_1}^{r_1^{-4}} y d(r^{-4})}{\int_{r_1}^{r_1^{-4}} d(r^{-4})} \quad (11)$$

It is an average of the non-dimensionalized specific volume over an inverse, cross-sectional area squared, coordinate. The integration is from the point behind the initial shock of the detonation zone where radial expansion ($r = 1$) begins to the CJ plane ($r = r_1$). When there is no radial expansion then the density at the CJ plane is found from the RUBY calculation to be 2.115 g/cm^3 . The density behind the shock (ρ_0) follows from combining an estimated shock Hugoniot of the powder with

the observed detonation velocity. It is about 2.4 g/cm^3 . If one assumes that, at the CJ plane, when lateral expansion has occurred the value of $\rho_i = 2.115$ decreased inversely as r_1^2 and then uses a linear average of densities, then $\bar{\gamma}$ is approximated by

$$\bar{\gamma} = \frac{\Delta}{\frac{1}{2} \left(\frac{\rho_i}{r_1^2} + \rho_0 \right)} = \frac{2\Delta}{\rho_0} \left[\frac{r_1^2}{\frac{\rho_i}{\rho_0} + r_1^2} \right] \quad (12)$$

An alternate approach is to approximate γ in Eq. 11 by having the density decrease from the value at $r = 1$ inversely proportional to r^2 . Integration of Eq. 11 then leads to

$$\bar{\gamma} = \frac{2\Delta}{\rho_0} \left[\frac{r_1^2}{1 + r_1^2} \right] \quad (13)$$

where $\Delta = 1.5$ and $\rho_0 = 2.4$

Numerical values for these two assumptions are listed below.

r_1^2 (area ratio)	1.1	1.5	2.0
$\bar{\gamma}$ from Eq. 12	0.6942	0.7876	0.8679
$\bar{\gamma}$ from Eq. 13	0.6548	0.7500	0.8333

In summary, Eq. 9, using the numerical values and relations for $\bar{\gamma}$ and b from the previous paragraphs, now gives U/U_0 in terms of r_1 . Further, from Eq. 8, we can find the corresponding pressure at the CJ plane and form the ratio to that for $r_1 = 1$. The values obtained are shown below together with the value of U that corresponds to a theoretical ideal detonation velocity (from RUBY) $U_0 = 4966 \text{ m/sec.}$

r_1^2	1.5	2.0	2.5	3.0	3.5	4.0	4.5
U_0/U	1.93	2.69	3.38	4.07	4.71	5.35	5.99
$U(\text{m/sec})$	2569	1848	1468	1221	1055	928	829
p_{r1}/p_1	0.294	0.155	0.098	0.067	0.050	0.039	0.031

It follows that for an experimentally observed detonation velocity of 928 m/sec the CJ plane is located where r_1^2 is 4, or $r_1 = 2$ and the pressure drops from the RUBY value for $r_1 = 1$ ($p_1 = 107$ kilobars) to 0.039 of it, that is, to 4.2 kilobars.

Designate by ℓ the distance measured away from the front, starting from the point where the area expansion of the reaction zone starts. Call the observed angle of this expansion, Θ and the cylindrical radial distance from the axis, d . Then for no expansion, $d = 0.5$ cm which is half the diameter of the explosive column. For the CJ plane it follows that

$$\tan \Theta = \frac{d - 0.5}{\ell} \quad r_1^2 = \frac{d^2}{(0.5)^2}$$

whence

$$\ell = \frac{0.5(r_1 - 1)}{\tan \Theta} \quad (14)$$

To use Eq. 14, the value of Θ , must be obtained from the observed reaction zone profiles. Figure 2 shows the variation in profiles observed for different loading conditions. For $\Theta = 30$ degrees Eq. 14 gives $\ell = 0.87$ cm which at 928 m/sec corresponds to 9.3 microsec.

DISCUSSION

The objective of the calculations presented herein was only to obtain an estimate of the location of the Chapman-Jouguet plane using the fact that the observed detonation velocity was one-fifth the theoretical ideal detonation velocity. It was recognized that the assumptions (discussed later) necessary to obtain a solution only supported the conclusion that the distance of the CJ plane, from the point where reaction commences is in the range of a fraction of a centimeter to a few centimeters. (0.87 cm was calculated corresponding to 9.3 microsec for a velocity of 928 m/sec).

It takes a minimum of 15 microsec to vaporize a 15 micron aluminum particle under the detonation zone conditions. (It is planned to treat the kinetics of aluminum particle vaporization in a separate report.) Thus, our calculation suggests incomplete combustion of the aluminum at the CJ plane, and supports the idea that physical kinetics is a significant factor in the detonation of a granular explosive.

Constraints on available fuel and associated chemical energy release were not included in the RUBY calculation of the ideal detonation velocity. To determine the effect of such constraints, the RUBY calculation was repeated with 33 and 67% of the aluminum available in the explosive made to appear as aluminum in the products. The explosive energy was altered correspondingly. Although numerical results were changed, the position of the CJ plane was still in the range of a fraction of a centimeter to a few centimeters.

The validity of the result depends on the assumptions made and the distributions associated with the numerical values used in the calculation. The quantities involved are (U/U_0) , Θ , \tilde{y} , b , b' , and k . U_0 and Θ have been observed in over fifty experiments. Some of these involved slightly different mixtures. It appears safe to say that Θ falls between 15 and 45 degrees (30 degrees was used) and that U_0 is between 800 and 1100 m/sec

(900 m/sec was used). U has been calculated for many variations of input conditions. U for conditions approximating the experiments and physical kinetics ranges from 4100 to 5800 s/sec (5000 m/sec was used). Hence, U/U_0 must fall between 4 and 7 (5 was used) and θ between 15 and 45 degrees (30 degrees was used).

The value of $k = C_v/R$ was a very slowly changing function of the RUBY explosive products. The key assumption believed correct, is that the condensed products contribute to specific heat, but not to the gas constant.

The value of b was first taken as constant and Jones formula used directly. The result was not much different than that presented herein for b a function of volume. However, the covolume calculated for the mixture that would exist at the CJ plane was double the constant value used in the calculation. It is for this reason that the calculation was redone for variable covolume. However, the fact that the results are similar for the two calculations indicates that b and b' variability is not a controlling factor.

The key \bar{y} assumption was that the density that exists at the CJ plane decreased inversely as the area ratio increased there. This ignores (for \bar{y} only) the effect on density of changes in particle velocity occasioned by the area increase. It was found that if \bar{y} was altered by $\pm 50\%$ in the equations with the other quantities in their normal range that the CJ location could be shifted in the range from 2 times to 1/3 the computed value.

Combining all the considerations of the above paragraphs it was decided that one could only conclude that the position of the CJ plane relative to the plane at which reaction commences was in the range of a fraction of a centimeter to a few centimeters. This is adequate to show that this granular medium confined in a Lucite tube has a detonation zone two magnitudes greater than that for a cast organic explosive. The long

detonation zone and information on fuel vaporization rates and observation of afterburning show that physical kinetics is a strong factor in the detonation.

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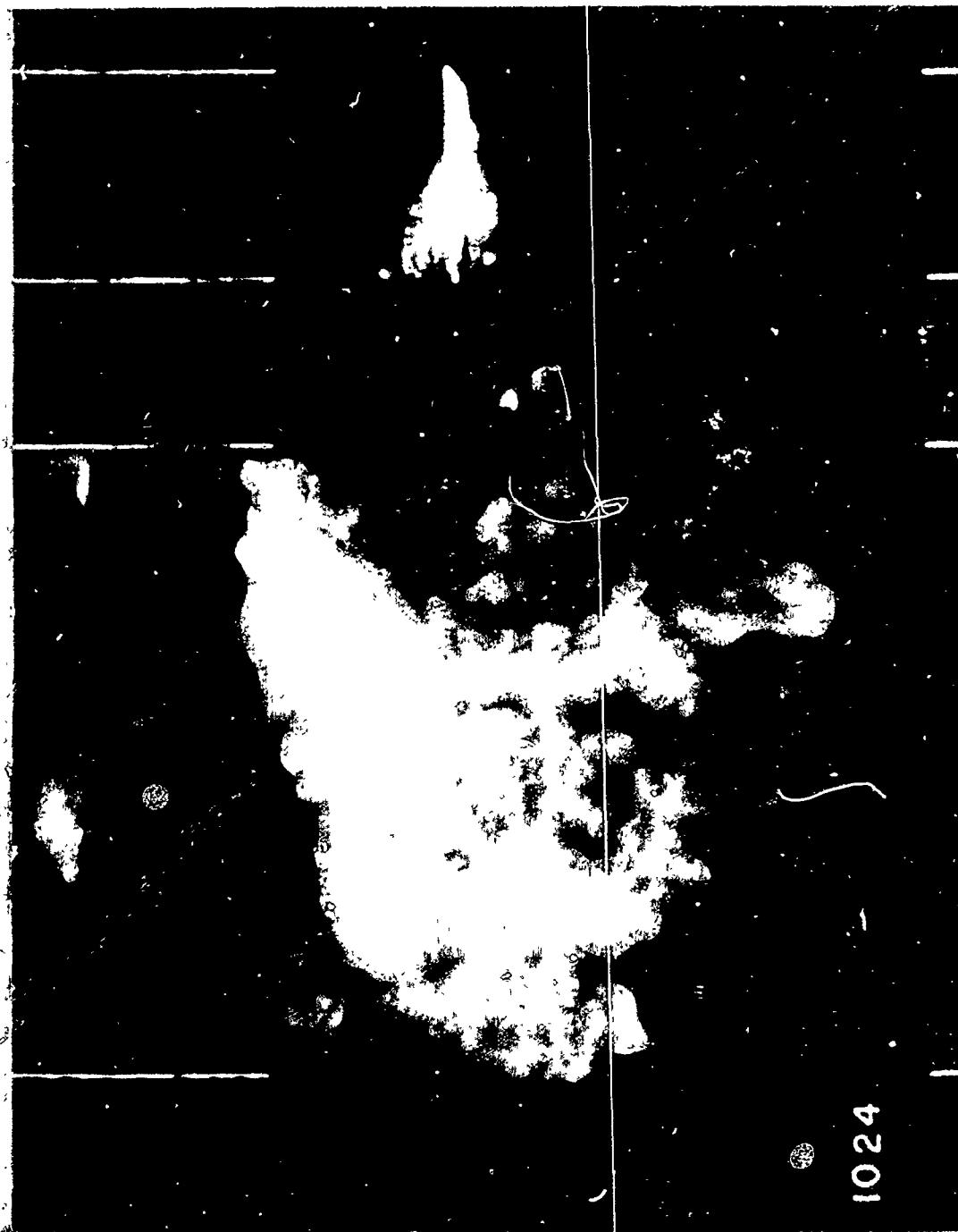


Fig. 1 Typical stable profile of the detonation of a granular mixture of potassium perchlorate and aluminum confined in a Lucite tube. The detonation velocity for this experiment (No. 1024) was 900 m/sec.

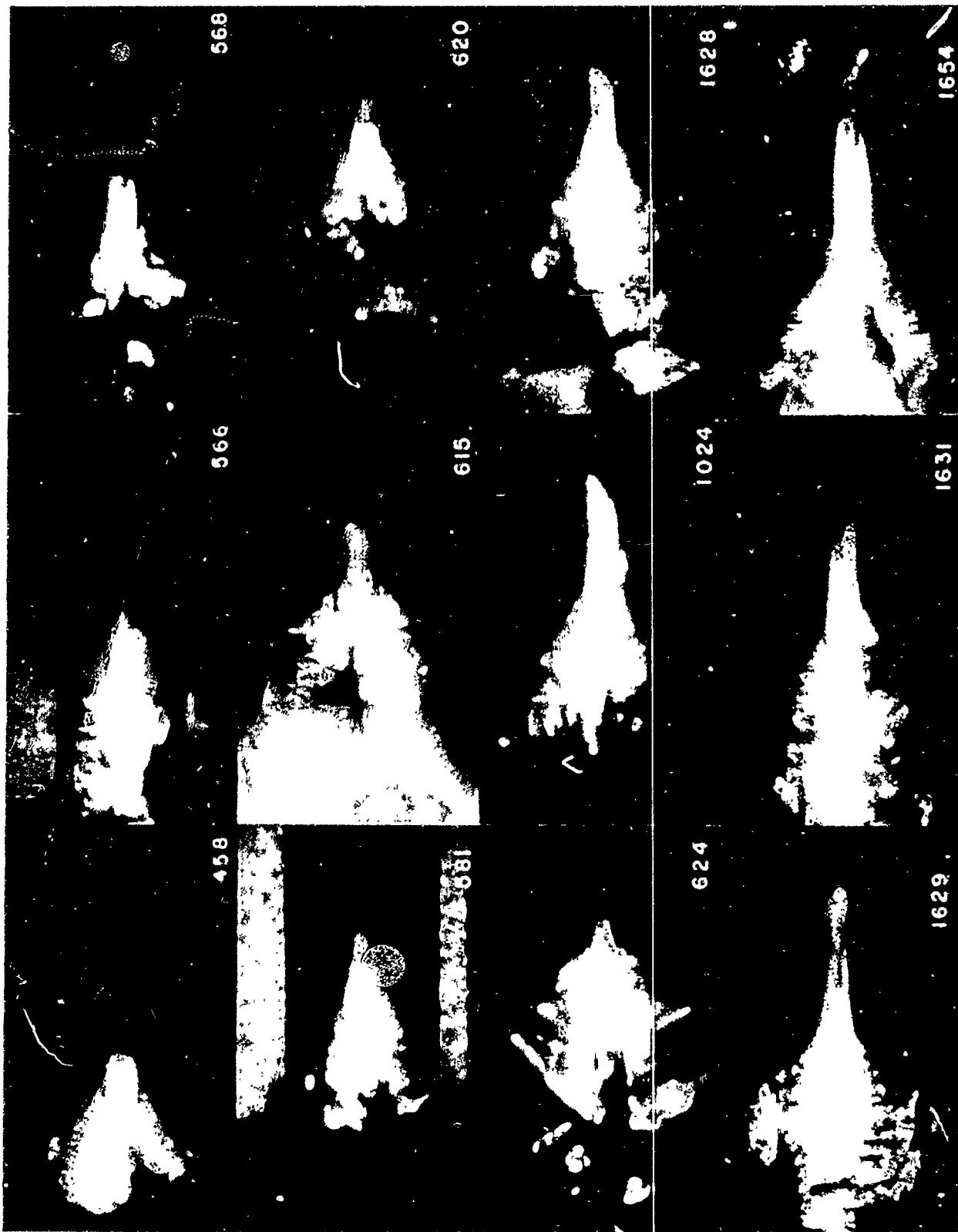


Fig. 2 Stable reaction zone profiles observed in different experiments on the detonation of a granular mixture of potassium perchlorate and aluminum confined in a Lucite tube. Numbers shown designate the experiments, not the detonation velocities.